Systematic Improvement of Splitting Methods for the Hamilton Equations

Asif Mushtaq, Anne Kværnø, and Kåre Olaussen

Abstract—We show how the standard (Störmer-Verlet) splitting method for differential equations of Hamiltonian mechanics (with accuracy of order τ^2 for a timestep of length τ) can be improved in a systematic manner without using the composition method. We give the explicit expressions which increase the accuracy to order τ^8, and demonstrate that the method work on a simple anharmonic oscillator.

Index Terms—Splitting-method, Hamilton-equations, Higher-order-accuracy, Symplecticity

I. INTRODUCTION

THE Hamilton equations of motion constitute a system of ordinary first order differential equations,

$$\dot{q}^a = \frac{\partial H}{\partial p_a}, \quad \dot{p}_a = -\frac{\partial H}{\partial q^a}, \quad a = 1, \ldots, N, \qquad (1)$$

where the ˙ denotes differentiation with respect to time t, and $H = H(\boldsymbol{q}, \boldsymbol{p})$. They can be viewed as the characteristic equations of the partial differential equation

$$\frac{\partial}{\partial t} \rho(\boldsymbol{q}, \boldsymbol{p}; t) = \mathcal{L} \rho(\boldsymbol{q}, \boldsymbol{p}; t), \qquad (2)$$

with $\mathcal{L}$ the first order differential operator

$$\mathcal{L} = \sum_{a=1}^{N} \frac{\partial H}{\partial p_a} \frac{\partial}{\partial q^a} - \frac{\partial H}{\partial q^a} \frac{\partial}{\partial p_a}, \qquad (3)$$

generating a flow on phase space. If H does not depend explicitly on t, a formal solution of (2) is

$$\rho(\boldsymbol{q}, \boldsymbol{p}; t) = \mathrm{e}^{t\mathcal{L}} \rho(\boldsymbol{q}, \boldsymbol{p}; 0). \qquad (4)$$

In most cases this expression remain just formal, but one may often split the Hamiltonian into two parts, $H = H_1 + H_2$, with a corresponding splitting $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$ such that the flows generated by $\mathcal{L}_1$ and $\mathcal{L}_2$ separately are integrable. One may then use the Cambell-Baker-Hausdorff formula to approximate the flow generated by $\mathcal{L}$. One obtains the Strang splitting formula [1], [2]

$$\mathrm{e}^{\frac{1}{2}\tau\mathcal{L}_2} \, \mathrm{e}^{\tau\mathcal{L}_1} \, \mathrm{e}^{\frac{1}{2}\tau\mathcal{L}_2} = \mathrm{e}^{\tau\mathcal{L} + \frac{1}{24}\tau^3 [2\mathcal{L}_1 + \mathcal{L}_2, [\mathcal{L}_1, \mathcal{L}_2]] + \cdots}, \qquad (5)$$

which shows that time stepping this expression with a timestep τ provides an approximation with relative accuracy of order τ^2, exactly preserving the symplectic property of the flow.

This corresponds to the symplectic splitting scheme of iterating the process of solving

$$\dot{q}^a = \frac{\partial H_2}{\partial p_a}, \quad \dot{p}_a = -\frac{\partial H_2}{\partial q^a}, \quad \text{for step } \frac{1}{2}\tau,$$

$$\dot{q}^a = \frac{\partial H_1}{\partial p_a}, \quad \dot{p}_a = -\frac{\partial H_1}{\partial q^a}, \quad \text{for step } \tau, \qquad (6)$$

$$\dot{q}^a = \frac{\partial H_2}{\partial p_a}, \quad \dot{p}_a = -\frac{\partial H_2}{\partial q^a}, \quad \text{for step } \frac{1}{2}\tau.$$

Here the last part of one iteration may be combined with the first part of the next, unless one deals with time dependent systems or wants to register the state of the system at the intermediate times.

¿From a practical point of view the most interesting property of this formulation is that it can be interpreted directly in terms of physical processes. For instance, for Hamiltonians $H(\boldsymbol{q}, \boldsymbol{p}) = T(\boldsymbol{p}) + V(\boldsymbol{q})$, a standard splitting scheme is to choose $H_1 = T$ and $H_2 = V$. In that case (6) corresponds to a collection of freely streaming particles receiving kicks at regular time intervals τ, these kicks being dependent of the positions $\boldsymbol{q}$ of the particles. I.e, we may think of the evolution as a collection of *kicks* and *moves* [3].

It is not clear that this is the best way to approximate or model the exact dynamics of the real system. For instance, why should the motion between kicks be the free streaming generated by $T(\boldsymbol{p})$? There are more ways to split the Hamiltonian into two integrable parts [4]; the best splitting is most likely the one which best mimics the physics of equation (1). Further, since this equation is not solved exactly by (6) for any finite value of τ we need not necessarily choose H_2 to be *exactly* $H - H_1$ as long as it approaches this quantity sufficiently fast as $\tau \to 0$. We will exploit this observation to improve the accuracy of the splitting scheme (6) in a systematic manner.

We are, of course, not the first trying to improve on the Störmer-Verlet splitting scheme. An accessible review of several earlier approaches can be found in reference [5]. Neri [6] has provided the general idea to construct symplectic integrators for Hamiltonian systems. Forest and Ruth [7] discussed the explicit fouth order method for the integration of Hamiltonian equations for the simplest non-trivial case. Yoshida [8] worked out a symplectic integrator for any even order, and Suzuki [9] presented the idea of how recursive construction of successive approximants may be extended to other methods.

II. HARMONIC OSCILLATORS

For a simple illustration of our idea consider the Hamiltonian

$$H(p, q) = \frac{1}{2} \left(p^2 + q^2 \right), \qquad (7)$$

whose exact evolution over a time interval τ is

$$\begin{pmatrix} q_{\mathrm{e}} \\ p^{\mathrm{e}} \end{pmatrix} = \begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}. \qquad (8)$$

Compare this with a *kick-move-kick* splitting scheme over the same time interval, with $H_{\mathrm{kick}} = \frac{1}{2}kq^2$ and $H_{\mathrm{move}} = \frac{1}{2}mp^2$, where k and m may depend on τ. One full iteration gives

$$\begin{pmatrix} q_{\mathrm{s}} \\ p^{\mathrm{s}} \end{pmatrix} = \begin{pmatrix} 1 - \frac{1}{2}mk\tau^2 & m\tau \\ -(1 - \frac{1}{4}km\tau^2)k\tau & 1 - \frac{1}{2}km\tau^2 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}. \qquad (9)$$

We note that by choosing

$$m = \frac{\sin\tau}{\tau} = 1 - \frac{1}{6}\tau^2 + \frac{1}{120}\tau^4 - \frac{1}{5040}\tau^6 + \cdots,$$
$$k = \frac{2}{\tau}\tan\frac{\tau}{2} = 1 + \frac{1}{12}\tau^2 + \frac{1}{120}\tau^4 + \frac{17}{20160}\tau^6 + \cdots, \qquad (10)$$

the exact evolution is reproduced. If we instead choose a *move-kick-move* splitting scheme, with $H_{\mathrm{move}} = \frac{1}{2}\bar{m}p^2$ and $H_{\mathrm{kick}} = \frac{1}{2}\bar{k}q^2$, one iteration gives

$$\begin{pmatrix} q_{\mathrm{s}} \\ p^{\mathrm{s}} \end{pmatrix} = \begin{pmatrix} 1 - \frac{1}{2}\bar{m}\bar{k}\tau^2 & (1 - \frac{1}{4}\bar{m}\bar{k})\bar{m}\tau \\ -\bar{k}\tau & 1 - \frac{1}{2}\bar{k}\bar{m}\tau^2 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}, \qquad (11)$$

which becomes exact if we choose

$$\bar{m} = \frac{2}{\tau}\tan\frac{\tau}{2}, \quad \bar{k} = \frac{\sin\tau}{\tau}. \qquad (12)$$

It should be clear that this idea works for systems of harmonic oscillators in general, i.e. for quadratic Hamiltonians of the form

$$H(\boldsymbol{q}, \boldsymbol{p}) = \frac{1}{2}\left(\boldsymbol{p}^T M \boldsymbol{p} + \boldsymbol{q}^T K \boldsymbol{q}\right), \qquad (13)$$

where M and K are symmetric matrices. For a choosen splitting scheme and step interval τ there are always modified matrices $M_\tau = M + \mathcal{O}(\tau^2)$ and $K_\tau = K + \mathcal{O}(\tau^2)$ which reproduces the exact time evolution. For systems where M and K are too large for exact diagonalization, but sparse, a systematic expansion of M_τ and K_τ in powers of τ^2 could be an efficient way to improve the standard splitting schemes.

III. NONLINEAR SYSTEMS

For a more general treatment we consider Hamiltonians of the form

$$H(\boldsymbol{q}, \boldsymbol{p}) = \frac{1}{2}\boldsymbol{p}^T M \boldsymbol{p} + V(\boldsymbol{q}). \qquad (14)$$

A series solution of the Hamilton equations in powers of τ is

$$q_{\mathrm{e}}^a = q^a + p^a\tau - \frac{1}{2}\partial^a V \tau^2 - \frac{1}{6}\partial^a(DV)\tau^3 + \mathcal{O}(\tau^4),$$

$$p_a^{\mathrm{e}} = p_a - \partial_a V \tau - \frac{1}{2}\partial_a(DV)\tau^2 \qquad (15)$$
$$+ \partial_a\left(\frac{1}{12}\bar{D}V - \frac{1}{6}D^2V\right)\tau^3 + \mathcal{O}(\tau^4)$$

Here we have introduced notation to shorten expressions,

$$\partial_a \equiv \frac{\partial}{\partial q^a}, \quad \partial^a \equiv M^{ab}\partial_b, \quad p^a \equiv M^{ab}p_b,$$
$$D \equiv p_a\partial^a, \quad \bar{D} \equiv (\partial_a V)\partial^a, \qquad (16)$$

where we employ the *Einstein summation convention*: An index which occur twice, once in lower position and once in upper position, are implicitly summed over all available

values. I.e, $M^{ab}\partial_b \equiv \sum_b M^{ab}\partial_b$ (we will generally use the matrix M to rise an index from lower to upper position). The corresponding result for the *kick-move-kick* splitting scheme is

$$q_{\mathrm{s}}^a = q^a + p^a\tau - \frac{1}{2}\partial^a V \tau^2 + \mathcal{O}(\tau^4),$$

$$p_a^{\mathrm{s}} = p_a - \partial_a V \tau - \frac{1}{2}\partial_a(DV)\tau^2 \qquad (17)$$
$$+ \partial_a\left(\frac{1}{8}\bar{D}V - \frac{1}{4}D^2V\right)\tau^3 + \mathcal{O}(\tau^4).$$

As expected it differs from the exact result in the third order, but the difference can be corrected by introducing second order generators

$$T_2 = -\frac{1}{12}D^2V\tau^2, \quad V_2 = \frac{1}{24}\bar{D}V\tau^2, \qquad (18)$$

to be used in respectively the *move* and *kick* steps. Specialized to a one-dimensional system with potential $V = \frac{1}{2}q^2$ this agrees with equation (10). With this correction the *kick-move-kick* splitting scheme agrees with the exact solution to 4th order in τ, but differ in the τ^5-terms. We may correct the difference by introducing fourth order generators,

$$T_4 = \frac{1}{720}\left(D^4 - 9\bar{D}D^2 + 3D\bar{D}D\right)V\tau^4,$$
$$V_4 = \frac{1}{480}\bar{D}^2V\tau^4. \qquad (19)$$

Specialized to a one-dimensional system with potential $V = \frac{1}{2}q^2$ this agrees with equation (10). With this correction the *kick-move-kick* splitting scheme agrees with the exact solution to 6th order in τ, but differ in the τ^7-terms. We may correct the difference by introducing sixth order generators,

$$T_6 = -\frac{1}{60480}\left(2\,D^6 - 40\,\bar{D}D^4 + 46\,D\bar{D}D^3\right.$$
$$\left. - 15\,D^2\bar{D}D^2 + 54\,\bar{D}^2D^2 - 9\,\bar{D}D\bar{D}D\right.$$
$$\left. - 42\,D\bar{D}^2D + 12\,D^2\bar{D}^2\right)V\tau^6$$

$$V_6 = \frac{1}{161280}\left(17\,\bar{D}^3 - 10\,\bar{D}_3\right)V\tau^6, \qquad (20)$$

where we have introduced

$$\bar{D}_3 \equiv (\partial_a V)(\partial_b V)(\partial_c V)\partial^a\partial^b\partial^c. \qquad (21)$$

Specialized to a one-dimensional system with potential $V = \frac{1}{2}q^2$ this agrees with equation (10). With this correction the *kick-move-kick* splitting scheme agrees with the exact solution to 8th order in τ, but differ in the τ^9-terms. One may continue the correction process, but this is probably well beyond the limit of practical use already.

IV. SOLVING THE *move* STEPS

Addition of extra potential terms $V \to V_{\mathrm{eff}} \equiv V + V_2 + V_4 + \dots$ is in principle unproblematic for solution of the *kick* steps. The equations,

$$\dot{q}^a = 0, \quad \dot{p}_a = -\partial_a V_{\mathrm{eff}}(\boldsymbol{q}), \qquad (22)$$

can still be integrated exactly, preserving the symplectic structure. The situation is different for the kinectic term $T \to T_{\mathrm{eff}} \equiv T + T_2 + T_4 + \cdots$, since it now leads to equations

$$\dot{q}^a = \frac{\partial}{\partial p_a}T_{\mathrm{eff}}(\boldsymbol{q}, \boldsymbol{p}), \quad \dot{p}_a = -\partial_a T_{\mathrm{eff}}(\boldsymbol{q}, \boldsymbol{p}), \qquad (23)$$

which is no longer straightforward to integrate exactly. Although the problematic terms are small one should make sure that the *move* steps preserve the symplectic structure exactly. Let q, p denote the positions and momenta just before the *move* step, and Q, P the positions and momenta just after. We construct a generating function [10]–[12] $G(q, P; \tau)$, with

$$Q^a = \frac{\partial G}{\partial P_a}, \quad p_a = \frac{\partial G}{\partial q^a}. \quad (24)$$

This preserves the symplectic structure; we just have to construct G to represent the *move* step sufficiently accurately. Consider first the case without the correction terms. The choice $G = q^a P_a + \frac{1}{2} P^a P_a \tau$ gives

$$Q^a = q^a + P_a \tau, \quad p_a = P_a, \quad (25)$$

which is the correct relation. Now add the T_2-term to the *move* step. To order τ^4 the exact solution of equation (23) becomes

$$Q^a = q^a + p_a \tau - \frac{1}{6} \partial^a DV \tau^3 - \frac{1}{24} \partial^a D^2 V \tau^4,$$
$$P_a = p_a + \frac{1}{12} \partial_a D^2 V \tau^3 + \frac{1}{24} \partial_a D^3 V \tau^4. \quad (26)$$

Compare this with the result of changing

$$G \to G - \frac{1}{12} \mathcal{D}^2 V \tau^3 - \frac{1}{24} \mathcal{D}^3 V \tau^4, \quad (27)$$

where $\mathcal{D} \equiv P_a \partial^a$. The solution of equation (24) change from the relations (25) to

$$Q^a = q^a + P^a \tau - \frac{1}{6} \partial^a \mathcal{D}V \tau^3 - \frac{1}{8} \partial^a \mathcal{D}^2 V \tau^4, \quad (28)$$
$$p_a = P_a - \frac{1}{12} \partial_a \mathcal{D}^2 V \tau^3 - \frac{1}{24} \partial_a \mathcal{D}^3 V \tau^4. \quad (29)$$

Since $\mathcal{D}$ is linear in P, equation (29) constitute a system of third order algebraic equation which in general must be solved numerically. This should usually be a fast process for small τ. An exact solution of this equation is required to preserve the symplectic structure, but this solution should also agree with the exact solution of (23) to order τ^4. This may be verified by perturbation expansion in τ. A perturbative solution of equation (29) is

$$P_a = p_a + \frac{1}{12} \partial_a D^2 V \tau^3 + \frac{1}{24} \partial_a D^3 V \tau^4 + \dots,$$

which inserted into (28) reproduces the full solution (26) to order τ^4.

This process can be systematically continued to higher orders. We write the transformation function as

$$G(\tau) = \sum_{n=0}^{\infty} G_n \tau^n, \quad (30)$$

and find the first terms in the expansion to be

$$G_0 = q^a P_a,$$
$$G_1 = \frac{1}{2} P^a P_a,$$
$$G_2 = 0,$$
$$G_3 = -\frac{1}{12} \mathcal{D}^2 V,$$
$$G_4 = -\frac{1}{24} \mathcal{D}^3 V,$$
$$G_5 = -\frac{1}{240} \left(3 \mathcal{D}^4 + 3 \bar{D} \mathcal{D}^2 - \mathcal{D} \bar{D} \mathcal{D} \right) V, \quad (31)$$
$$G_6 = -\frac{1}{720} \left(2 \mathcal{D}^5 + 8 \bar{D} \mathcal{D}^3 - 5 \mathcal{D} \bar{D} \mathcal{D}^2 \right) V,$$
$$G_7 = -\frac{1}{20160} \left(10 \mathcal{D}^6 + 10 \bar{D} \mathcal{D}^4 + 90 \mathcal{D} \bar{D} \mathcal{D}^3 - 75 \mathcal{D}^2 \bar{D} \mathcal{D}^2 \right.$$
$$+ 18 \bar{D}^2 \mathcal{D}^2 - 3 \bar{D} \mathcal{D} \bar{D} \mathcal{D} - 14 \mathcal{D} \bar{D}^2 \mathcal{D} + 4 \mathcal{D}^2 \bar{D}^2) V,$$
$$G_8 = -\frac{1}{40320} \left(3 \mathcal{D}^7 - 87 \bar{D} \mathcal{D}^5 + 231 \mathcal{D} \bar{D} \mathcal{D}^4 - 133 \mathcal{D}^2 \bar{D} \mathcal{D}^3 \right.$$
$$+ 63 \bar{D}^2 \mathcal{D}^3 - 3 \mathcal{D} \bar{D}^2 \mathcal{D}^2 - 21 \mathcal{D}^2 \bar{D}^2 \mathcal{D} + 4 \mathcal{D}^3 \bar{D}^2$$
$$- 63 \bar{D} \mathcal{D} \bar{D} \mathcal{D}^2 + 25 \mathcal{D} \bar{D} \mathcal{D} \bar{D} \mathcal{D}) V.$$

V. Explicit Computations
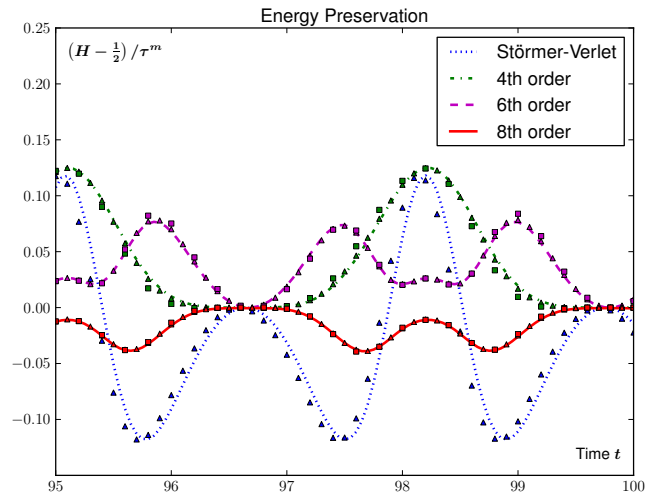

Fig. 1. This figure illustrate how well energy is conserved with the various splitting schemes. The quanties plotted is $(H - \frac{1}{2})/\tau^m$ for $\tau = 0.2$ (squares), $\tau = 0.1$ (triangles) and $\tau = 0.05$ (lines). Here $m = 2$ for the Störmer-Verlet scheme (dotted line), $m = 4$ for the τ^2-corrected generators (dash-dotted line), $m = 6$ for the τ^4-corrected generators (dashed line), and $m = 8$ for the τ^6-corrected generators (fulldrawn line). Each plotted quantity is essentially the value of the next correction at the visited point in phase space. Since the plot is taken over the last half of the 16th period the figure also give some indication of how well the exact oscillation period is reproduced by the scheme. The deviation is quite large for the Störmer-Verlet scheme when $\tau = 0.2$; to avoid cluttering the figure we have not included these points.

It remains to demonstrate that our algorithms can be applied to real examples. We have considered the Hamiltonian

$$H = \frac{1}{2} p^2 + \frac{1}{4} q^4, \quad (32)$$

with initial condition $q(0) = 0$, $p(0) = 1$. The exact motion is a nonlinear oscillation with H constant equal to $\frac{1}{2}$, and period

$$T = 4 \int_0^{2^{1/4}} \frac{\sqrt{2}\,dq}{\sqrt{2 - q^4}} = 2^{1/4} B(\frac{1}{4}, \frac{1}{2}) \approx 6.236\,339\dots. \quad (33)$$

Here $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$ is the beta function. In figure 1 we plot the behaviour of $\left(H - \frac{1}{2}\right)/\tau^{2+n}$ during the last half of the 16th oscillation, for various values of τ and corrected generators up to order τ^6 (corresponding to $n = 6$).
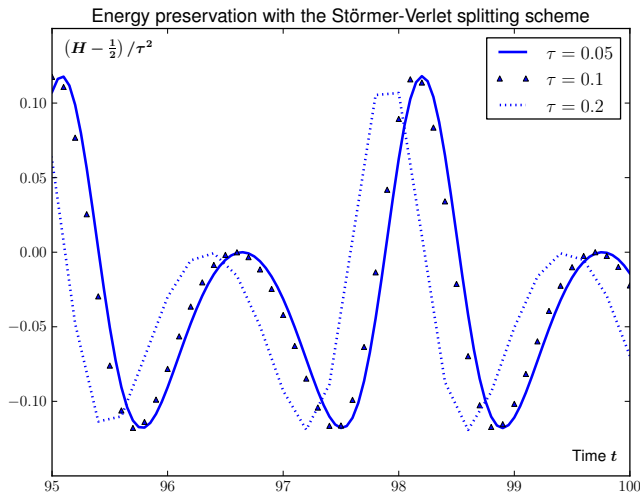

Fig. 2. This figure illustrate the long time behaviour (through the last half of the 16th period) for the Störmer-Verlet scheme. Different timesteps τ have an effect on the period of oscillation, but the preservation of energy remains stable for a very long time.
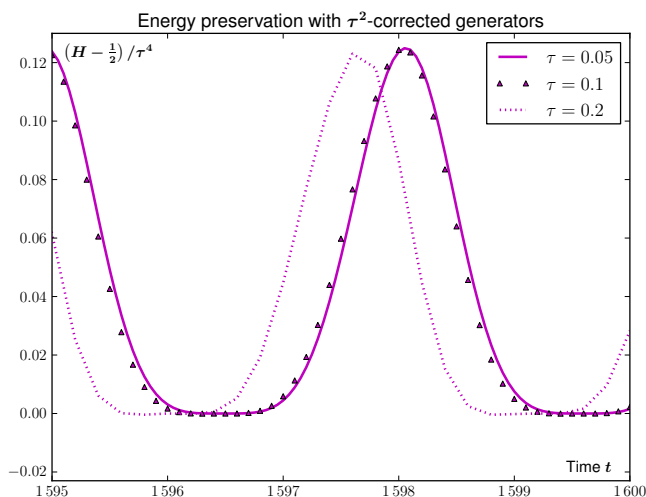

Fig. 3. This figure illustrate the long time behaviour (through the first half of the 257th period) for the τ^2-corrected scheme. Different timesteps τ have an effect on the period of oscillation, but the preservation of energy remains stable for a very long time.

VI. Conclusion

We have shown that it is possible to systematically improve the accuracy of the usual symplectic integration schemes for a rather general class of Hamilton equations. The process is quite simple for linear equations, where it may be useful for sparse systems. For general systems the method requires the solution of a set of nonlinear algebraic equations at each *move* step. To which extent an higher-order method is advantageous or not will depend on the system under analysis, and the wanted accuracy. As always with higher order methods the increased accuracy per step may be countered by the higher computational cost per step [13].
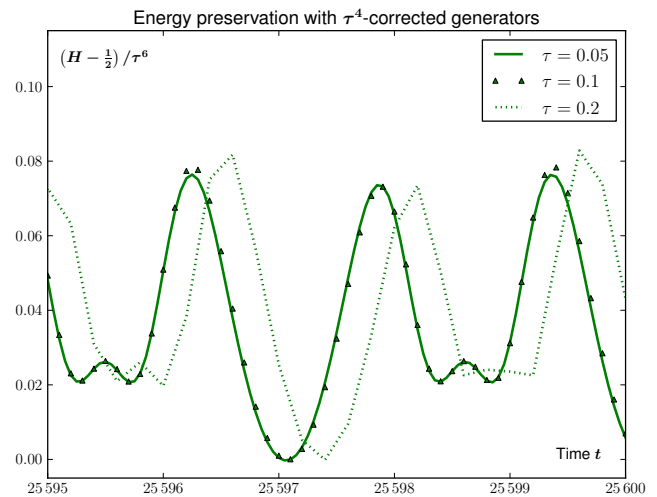

Fig. 4. This figure illustrate the long time behaviour for the τ^4-corrected scheme (through the last half of the $4\,104^{\text{th}}$ period). Different timesteps τ have an effect on the period of oscillation, but the preservation of energy remains stable for a very long time.
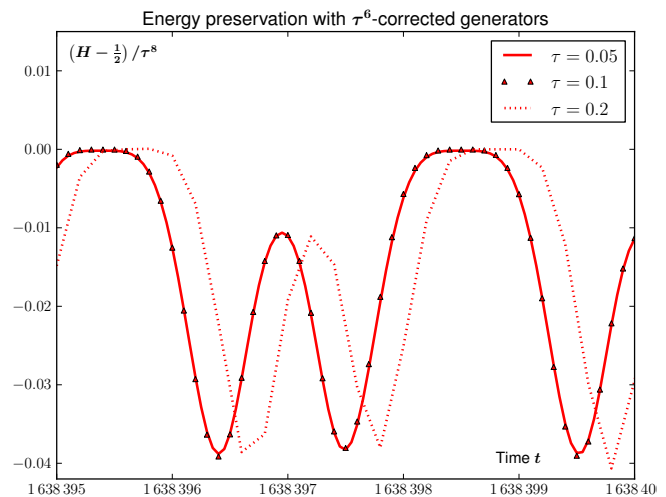

Fig. 5. This figure illustrate the long time behaviour for the τ^6-corrected scheme (through the last half of period $262\,718$). Different timesteps τ have an effect on the period of oscillation, but the preservation of energy remains stable for a very long time (for high accuracy and very long runs the effect of numerical roundoff errors eventually becomes visible).

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